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The comparison in Table III of our density functional theory results to previous *ab initio* results for the hyperpolarizabilities of para-nitroaniline (PNA) is incorrect. As for the other systems discussed in our paper, we used a convention based on a Taylor series expansion of the dipole moment (this is convention T or AB in the terminology of Ref. 1). It was, however, overlooked that a different convention was used for the *ab initio* PNA results (convention B in Ref. 1) to which we compare. The present table replaces Table III.

TABLE I. Static and frequency-dependent average hyperpolarizabilities of para-nitroaniline at $\lambda=1060$ nm ($\omega=0.043$ a.u.), using convention B of Ref. 1.

Property	LDA/ALDA[a]	LB94/ALDA[a]	HF[b]	MP2[c]
$\beta_{\mathrm{vec}}(0;0,0)$[d]	7.45	8.14	4.37	8.55
$\beta_{\mathrm{vec}}(-2\omega;\omega,\omega)$[d]	16.99	21.16	4.88	12.0
$\overline{\gamma}(0;0,0,0)$[e]	1.22	0.44	1.48	3.21
$\overline{\gamma}(-2\omega;\omega,\omega,0)$[e]	3.36	2.00	2.11	4.6

[a]This work, using ALDA for functional derivatives of v_{xc}, and either LDA or LB94 for v_{xc} itself.
[b]Reference 3.
[c]Results obtained by Sim *et al.*,[2] frequency dispersion was estimated from TDHF calculation.
[d]$\beta_{\mathrm{vec}}=\beta_z=(1/3)\Sigma_a\beta_{zaa}+\beta_{aza}+\beta_{aaz}$, given in units of 10^{-30} esu, as in Refs. 3, 4, 2.
[e]$\overline{\gamma}=(1/15)\Sigma_{a,b}(2\gamma_{aabb}+\gamma_{abba})$, in 10^{-36} esu, as in Ref. 3.

Our previous LDA/ALDA and LB94/ALDA numbers have been divided by a factor of two for the β-values and a factor of six for the γ-values, so that all numbers in the PNA table are now in convention B.

The $\beta_{zzz}(0;0,0)$ value of -1959 a.u. quoted in the text on p. 10655 should be replaced by $+1959$ a.u. in convention AB (the sign should be positive because the hyperpolarizability is parallel to the dipole moment, not antiparallel), or 980 a.u. in convention B.

The lines ''Both the $\beta(-2\omega;\omega,\omega)\ldots$ than in those papers, which $\ldots$'' near the end of p. 10655 should be replaced by ''The frequency dependence is substantially higher than in the *ab initio* results, which $\ldots$''.

These corrections do not affect the theoretical discussion of calculating dynamic hyperpolarizabilities in density functional theory nor the discussion of the tests on the correctness of our implementation, which formed the central issues of the paper.

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